



Glenn T. Seaborg Center Seminar

Quantum Chemistry Applied to Actinides: Methods, Mineral Surfaces, Macrocycles and Other Systems

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**Wednesday, July 9, 2014
4:00 pm – 5:00 pm
Bldg. 70A, Room 3377**

The chemistry of the early actinide elements is an area of chemistry that is particularly conducive to collaborations between experimental and theoretical research, due to the inherent challenges presented by this part of the periodic table. In this talk, I will discuss some of those challenges on the theoretical side, along with other methodological aspects. This will be followed by some stories from our recent research. I will use them to illustrate the type of problems that may be addressed, as well as the unique answers that computational chemistry can provide. Specifically, we will focus on the following:

- Aqueous chemistry – plutonyl hydroxide complexes;
- Predicting novel species and bonding schemes – the “pacman” system;
- Mineral surfaces – uranyl interaction with TiO_2 surfaces.

In each case, I will attempt to draw specific as well as general conclusions regarding the methodology employed and the chemistry involved.